LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100194.D
Acq On : 4 Nov 2017 22:17
Operator : SJ/JU
Sample : I6313-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF019-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.787	285	289	312	rBV	30800	70798	3.64%	0.432%
2	4.987	489	493	515	rBV	112283	220687	11.35%	1.347%
3	5.392	559	562	589	rBV	968685	1492650	76.76%	9.111%
4	6.416	733	736	754	rBV	1243490	1547181	79.57%	9.444%
5	6.539	754	757	773	rVB	1613441	1669001	85.83%	10.188%
6	6.763	792	795	808	rBV	504263	479371	24.65%	2.926%
7	6.916	818	821	839	rBV	1368247	1284699	66.07%	7.842%
8	7.334	889	892	917	rBV	849455	943540	48.52%	5.759%
9	8.045	1010	1013	1031	rBV	690371	682185	35.08%	4.164%
10	9.116	1191	1195	1210	rBV	2226259	1944461	100.00%	11.869%
11	9.516	1260	1263	1275	rBV	138252	130537	6.71%	0.797%
12	9.798	1307	1311	1323	rVB	835489	791698	40.72%	4.833%
13	10.592	1443	1446	1460	rBV	1138926	1112145	57.20%	6.789%
14	11.286	1561	1564	1574	rBV	816015	806132	41.46%	4.921%
15	11.804	1649	1652	1662	rBV2	60722	67365	3.46%	0.411%
16	12.586	1781	1785	1793	rBV	28358	39375	2.02%	0.240%
17	12.868	1829	1833	1836	rBV	2147714	1924002	98.95%	11.744%
18	13.739	1978	1981	1990	rVB	47653	56052	2.88%	0.342%
19	13.939	2012	2015	2024	rBV	629364	626481	32.22%	3.824%
20	14.657	2133	2137	2141	rBV2	44574	48035	2.47%	0.293%
21	15.398	2259	2263	2279	rBV	288269	446122	22.94%	2.723%

Sum of corrected areas: 16382517

LSC Report - Integrated Chromatogram

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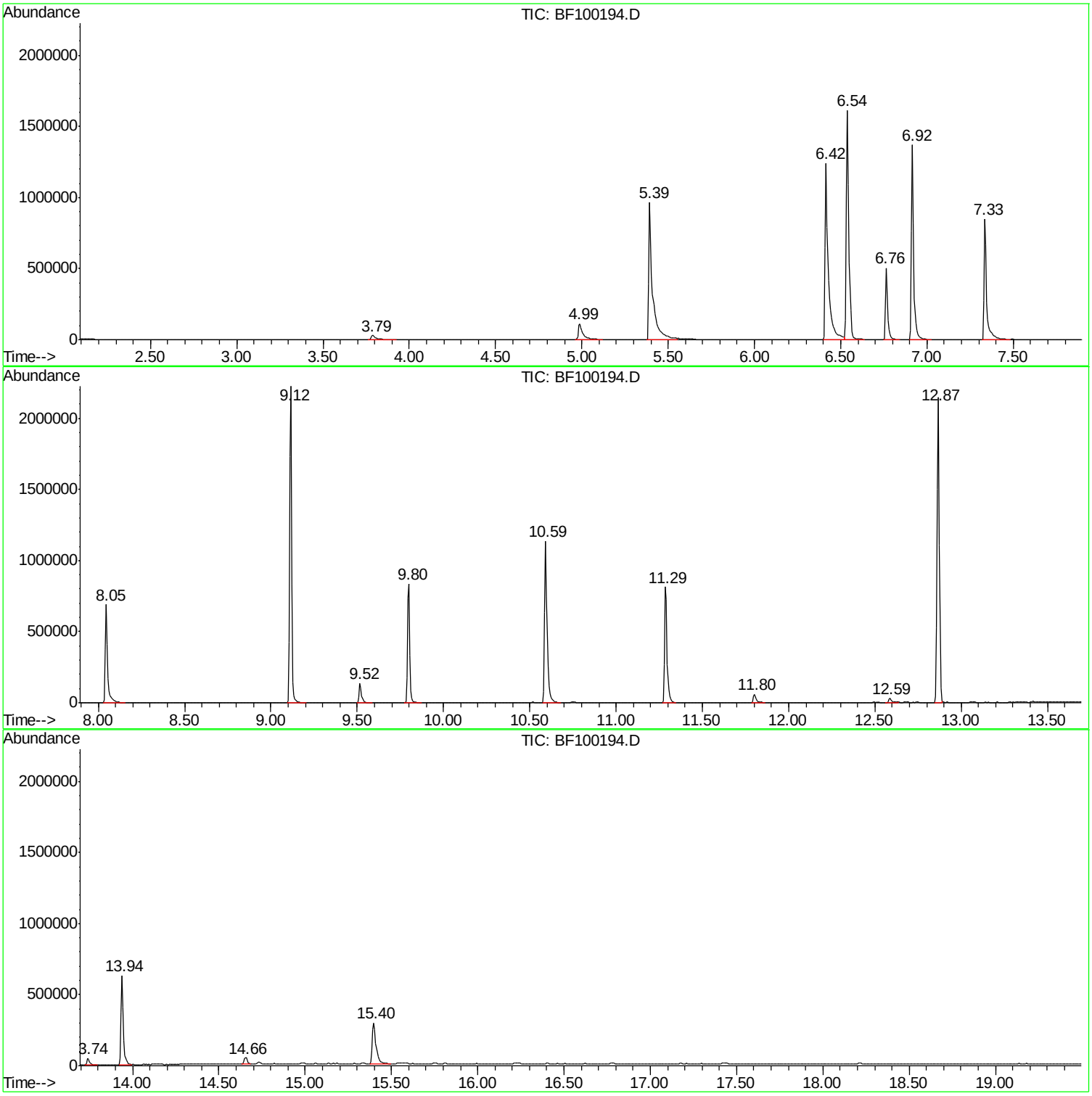
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : BF100194.D
Acq On : 4 Nov 2017 22:17
Operator : SJ/JU
Sample : I6313-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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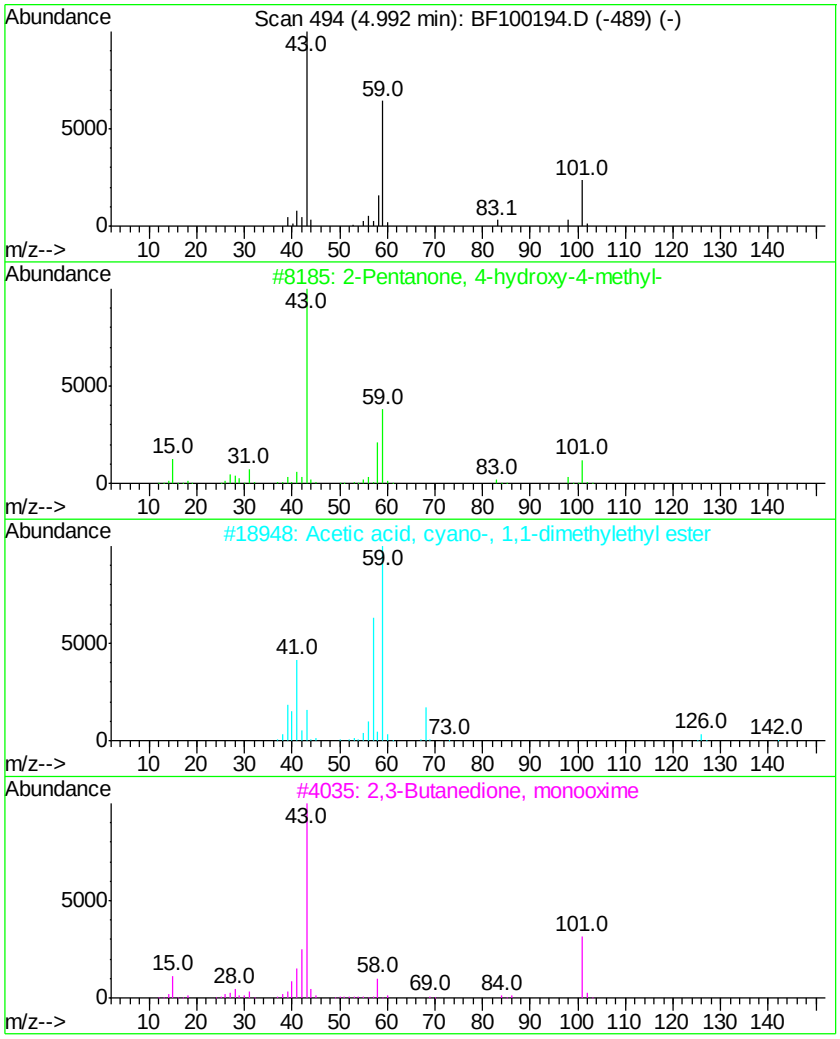
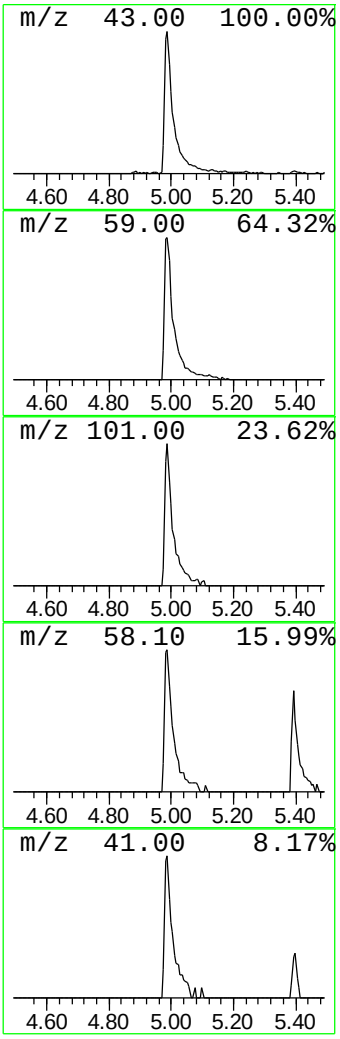
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	9.21 ng	220687	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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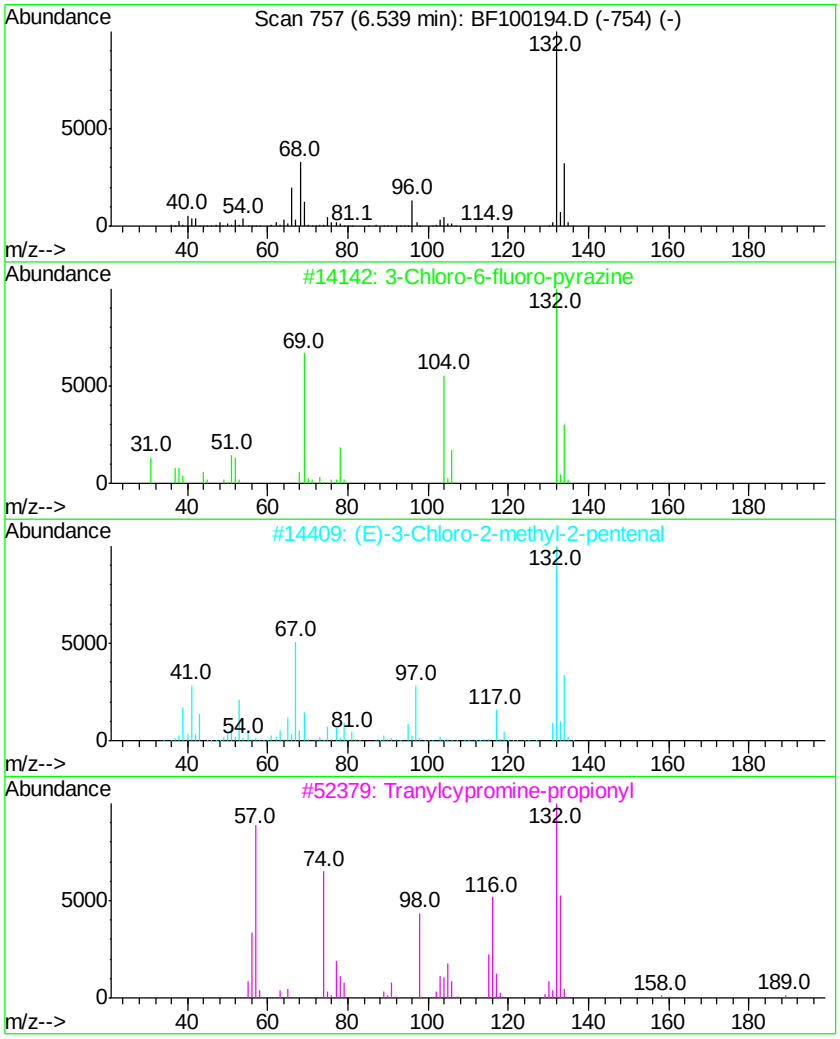
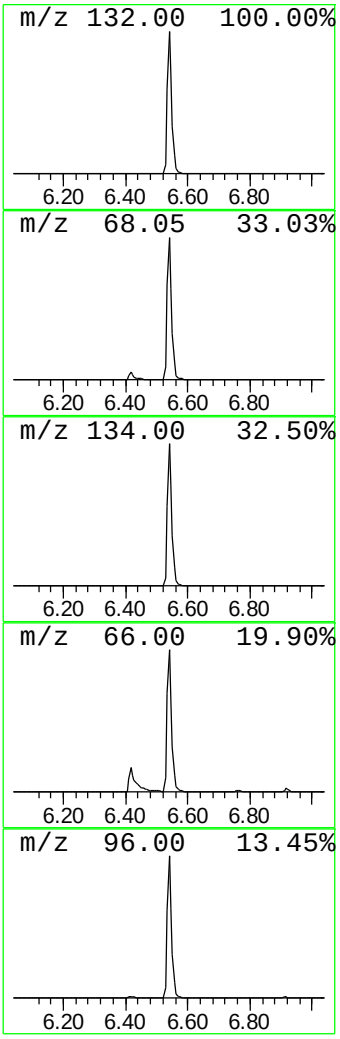
Peak Number 3 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	69.63 ng	1669000	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	9.2	ng	220687	1	6.76	479371	20.0
unknown6.54	6.54	69.6	ng	1669000	1	6.76	479371	20.0